APPENDIX B

SUPPORTING INFORMATION FOR HYDROGEOLOGIC MODELING

B-1 Review of Groundwater Modeling Codes and their Application for Permeable Barriers

B-2 Illustrations of the Hydrologic Modeling Approach for Permeable Barrier Application

APPENDIX B-1
GROUNDWATER FLOW MODEL REVIEW

This appendix presents the general concepts of groundwater flow modeling and describes several modeling codes that may be used in designing and evaluating the permeable barrier systems.

GROUNDWATER FLOW MODELING CONCEPTS

To aid in the design of a permeable barrier system and the interpretation of the resulting flow field, it is recommended that a groundwater flow model be constructed using the site-specific geologic and hydrogeologic data collected as part of the site characterization effort. The model can be used to assess the area of influence, optimize the design, and design the performance monitoring network for the permeable barrier system. A complete description of groundwater flow modeling and the mathematics involved is provided in Wang and Anderson (1982) and Anderson and Woessner (1992). The steps involved in model construction and execution are discussed below.

Conceptual Model Development

The first step in any modeling effort is the development of the conceptual model. The conceptual model is a three-dimensional representation of the groundwater flow and transport system based on all available geologic, hydrogeologic, and geochemical data for the site. A complete conceptual model will include geologic and topographic maps of the site, cross sections depicting the site geology/hydrogeology, a description of the physical and chemical parameters associated with the aquifer(s), and contaminant concentration and distribution maps. The purpose of the conceptual model is the integration of the available data into a coherent representation of the flow system to be modeled. The conceptual model is used to aid in model selection, model construction, and interpretation of model results.

Model Selection

In order to be used to simulate the flow at permeable barriers, the groundwater flow model requires several special features/capabilities. The most important requirements derive from the need to simulate sharp hydraulic conductivity (K) contrasts at the intersection of the aquifer and the funnel walls. The specific requirements and recommendations for the permeable barrier simulation models include:

- Two-dimensional or three-dimensional groundwater flow models may be used to simulate the flow system of a site under consideration. A three-dimensional modeling approach is recommended so that the possibility of underflow or overflow and of interactions between the adjacent aquifer can be examined at the permeable barrier and its vicinity. Vertical-flow velocities and travel times will be of critical significance in the design of systems at sites with significant vertical-flow gradients or in cases where the barriers are not keyed into the underlying confining layer.

- The codes should be able to simulate large contrasts in K at the funnel walls. Most of the permeable barrier designs include a reactive cell with K higher that that of the aquifer and flanking funnel walls with extremely low permeability. The funnels may consist of the slurry wall, which can be several feet wide, or the sheet piles, which are usually less than an inch in width. Therefore, at the intersection of the aquifer and the reactive cells, large K contrasts are developed, and many models are unable to solve these problems due to numerical instabilities. In most cases, the funnel walls are simulated by assigning a very low conductivity to the model cells representing the funnel locations. For accurate simulations, the size of these funnel cells should be the same as that of slurry walls. This results in a very small cell size and a large number of cells in the model. The sheet piles are even thinner than the slurry walls and the required cell sizes may be even smaller. To simulate large areas with sufficient resolution near the funnels but larger cells away from the funnels, models capable of incorporating grid blocks of variable size are recommended. Some alternative approaches have been devised to simulate the low-K funnel walls. These are discussed with the appropriate model descriptions in the "Permeable Barrier Simulation Models" section below.

- Many sites have significant heterogeneities, which result in the development of preferential pathways through which most of the groundwater movement occurs. The permeable barrier design itself imparts heterogeneity to the subsurface system. The simulation of these effects requires models that can handle heterogeneity. Most general-purpose analytical models are based on the assumption of homogeneity, but most numerical models can incorporate heterogeneities.

- Many sites have features such as streams, drains, tunnels, or wells in the vicinity of the permeable barrier sites. For example, at some sites, pump-and-treat remediation may be active in the vicinity of the permeable barriers. These situations require the use of models that can simulate the effects of these internal sinks or sources on the permeable barrier systems.

- The results of the model should be amenable to use with the particle-tracking programs so that the capture zones of the permeable barriers can be evaluated. It should also be possible to calculate volumetric flow budgets for the reactive cells.

Many groundwater flow modeling codes currently on the market meet the above requirements. A comprehensive description of nonproprietary and proprietary flow-and-transport modeling codes can be found in the U.S. Environmental Protection Agency document entitled *Compilation of Ground-Water Models* (van der Heijde and Elnawawy, 1993). Depending on the project's needs, the designer of a permeable barrier system may want to apply a contaminant transport code that can utilize the calculated hydraulic-head distribution and flow field from the flow-modeling effort. If flow and transport in the vadose zone are of concern, a coupled or uncoupled, unsaturated/saturated flow and transport model should be considered. The intention of this protocol is not to endorse a specific code, but to suggest a nonproprietary code (that may also be provided privately) that will serve as an example of the type of modeling code that should be used. The proprietary codes are mentioned only if they have been used to simulate the permeable barrier system at a site. The codes that meet most of the requirements for simulation of permeable barrier systems are discussed in the "Permeable Barrier Simulation Models" section below.

Model Construction and Calibration

Model construction consists primarily of converting the conceptual model into the input files for the numerical model. The hydrostratigraphic units defined in the conceptual model can be used to define the physical framework or grid mesh of the numerical model. In both finite-difference (such as MODFLOW) and finite-element models, a model grid is constructed to discretize the lateral and vertical space that the model is to represent. The different hydrostratigraphic units are represented by model layers, each of which is defined by an array of grid cells. Each grid cell is defined by hydraulic parameters (e.g., K, storativity, cell thickness, cell top, bottom) that control the flow of water through the cells.

Model boundaries are simulated by specifying boundary conditions that define the head or flux of water that occurs at the model grid boundaries or edges. Boundary conditions describe the interaction between the system being modeled and its surroundings. Boundary conditions are used to include the effects of the hydrogeologic system outside the area being modeled and also to make possible isolation of the desired model domain from the larger hydrogeologic system. Three types of boundary conditions generally are utilized to describe groundwater flow: specified-head (Dirichlet), specified-flux (Neumann), and head-dependent flux (Cauchy) (Anderson and Woessner, 1992). Internal boundaries or hydrologic stresses, such as wells, rivers, drains, and recharge, may also be simulated using these conditions.

Calibration of a groundwater flow model refers to the demonstration that the model is capable of producing field-measured heads and flows, which are used as the calibration values or targets. Calibration is accomplished by finding a set of hydraulic parameters, boundary conditions, and stresses that can be used in the model to produce simulated heads and fluxes that match field-measured values within a pre-established range of error (Anderson and Woessner, 1992). Model calibration can be evaluated through statistical comparison of field-measured and simulated conditions.

Model calibration often is difficult because values for aquifer parameters and hydrologic stresses typically are known in relatively few locations and their estimates are influenced by uncertainty. The uncertainty in a calibrated model and its input parameters can be evaluated by performing a sensitivity analysis in which the aquifer parameters, stresses, and boundary conditions are varied within an established range. The impact of these changes on the model output (or hydraulic heads) provides a measure of the uncertainty associated with the model parameters, stresses, and boundary conditions used in the model. To ensure a reasonable representation of the natural system, it is important to calibrate with values that are consistent with the field-measured heads and hydraulic parameters. Calibration techniques and the uncertainty involved in model calibration are described in detail in Anderson and Woessner (1992).

Model Execution

After a model has been calibrated to observed conditions, the model can be used for interpretive or predictive simulations. In a predictive simulation, the parameters determined during calibration are used to predict the response of the flow system to future events, such as the decrease in K over time or the effect of pumping in the vicinity of the permeable barrier. The predictive requirements of the model will determine the need for either a steady-state simulation or a transient simulation, which would accommodate changing conditions and stresses through time. Model output and hydraulic heads can be interpreted through the use of a contouring package and should be applied to particle-tracking simulations to calculate groundwater pathways, travel times, and fluxes through the cell. Establishing travel times through the cell is a key modeling result that can be used to determine the thickness of the permeable cell.

PERMEABLE BARRIER SIMULATION MODELS

This section describes the various computer simulation codes that meet the minimum requirements for simulations of groundwater flow and particle movement at the permeable barrier sites. Some of the codes already have been used at permeable barrier sites. Nearly all are readily available from the authors or their sponsoring agencies or through resellers. Proprietary codes are included only if they have been applied at a permeable barrier site. Not discussed are advanced programs, such as HST3D (Kipp, 1987), that can simulate the groundwater flow in the vicinity of permeable barriers, but are in fact designed for simulation of more complex processes.

MODFLOW and Associated Programs

Perhaps the most versatile, widely used, and widely accepted groundwater modeling code is that of the U.S. Geological Survey modular, three-dimensional, finite-difference, groundwater flow model, commonly referred to as MODFLOW (McDonald and Harbaugh, 1988). MODFLOW simulates two-dimensional and quasi- or fully three-dimensional, transient groundwater flow in anisotropic, heterogeneous, layered aquifer systems. MODFLOW calculates piezometric head distributions, flow rates, and water balances; it includes modules for flow toward wells, through riverbeds, and into drains. Other modules handle evapotranspiration and recharge. There are available on the market various textual and graphical pre- and postprocessors that make it easy to use the code and analyze the simulation results. These include GMS (Groundwater Modeling System) (Brigham Young University, 1996), ModelCad (Rumbaugh, 1993), Visual MODFLOW (Waterloo Hydrogeologic, Inc., 1996), and Groundwater Vistas (Environmental Simulations, Inc., 1994).

Additional simulation modules are available through the authors and third parties. One of these is the Horizontal Flow Barrier (HFB) package (Hsiech and Freckleton, 1993). It is especially useful in simulating the funnel-and-gate design. In normal cases, the slurry walls have to be simulated by very small cells of low K, increasing the number of cells in the model dramatically. The HFB package permits the user to assign the sides of certain cells as planes of low K, while still using a larger cell size at the funnel walls. The low-conductivity HFB planes restrict the flow of water into the cells across the faces representing slurry walls or sheet piles. Another useful addition is the ZONEBUDGET (Harbaugh, 1990) package, which allows the user to determine the flow budget for any section of the model. This package may be used to evaluate the volumetric flow through the cell for various design scenarios.

The results from MODFLOW can be used in particle-tracking codes, such as MODPATH (Pollock, 1989) and PATH3D (Zheng, 1989), to calculate groundwater paths and travel times. MODPATH is a postprocessing package used to compute three-dimensional groundwater path lines based on the output from steady-state simulations obtained with the MODFLOW modeling code. MODPATH uses a semi-analytical, particle-tracking scheme, based on the assumption that each directional velocity component varies linearly within a grid cell in its own coordinate direction. PATH3D is a general particle-tracking program for calculating groundwater paths and travel times in transient three-dimensional flow fields. The program includes two major segments - a velocity interpolator, which converts hydraulic heads generated by MODFLOW into a velocity field, and a fourth-order Runge-Kutta numerical solver with automatic time-step size adjustment for tracking the movement of fluid particles (van der Heijde and Elnawawy, 1993). A proprietary code, RWLK3D, developed by Battelle (Naymik and Gantos, 1995), also has been used in conjunction with MODFLOW to simulate the particle movement for the pilot-scale permeable cell installed at Moffett Federal Airfield (Battelle, 1996a). This is a 3-dimensional transport and particle-tracking code based on the Random Walk approach to solute transport simulation.

FLOWPATH

FLOWPATH (Waterloo Hydrogeologic, Inc., 1996) is a 2D, Steady-state, groundwater flow and pathline model. The code can simulate confined, unconfined, or leaky aquifers in heterogeneous and anisotropic media. Complex boundary conditions can be simulated. The program output includes simulated hydraulic heads, pathlines, travel times, velocities, and water balances. The funnel walls can be simulated by constructing a model grid with very small cell size in the vicinity of the permeable cells. Because of its user-friendly graphical interface, this program can be used to quickly simulate the flow fields for a number of design options. Therefore, this program has been used for several permeable barrier sites. However, this program cannot be used if the groundwater flow at a site is very complex due to vertical fluxes or if transient flow fields are to be simulated. These situations are possible if there is a potential for vertical underflow or if the permeable wall is not keyed into the confining layer.

FRAC3DVS

FRAC3DVS is a 3D, finite-element model for simulating steady-state or transient, saturated or variably saturated, groundwater flow and advective-dispersive solute transport in porous or discretely fractured porous media. The code was developed at the University of Waterloo (Therrien, 1992 and Therrien and Sudicky, 1995) and is being marketed by Waterloo Hydrogeologic, Inc. The code includes preprocessors for grid mesh and input file generation and postprocessors for visualization of the simulation results. This program has many advanced features that are generally not required for simple permeable barrier designs. However, it is included here because the code has been used by Schikaze (1996) to simulate a hypothetical funnel-and-gate design. Further, the solute transport features of this code include the ability to simulate the multispecies transport of straight or branching decay chains. This feature may be used to simulate the reaction progress and daughter product generation in the sequential decay of chlorinated solvents in the permeable cells.

In the work by Schikaze, the impermeable cutoff walls are implemented as 2D planes within the 3D computational domain. This is done by adding “false nodes” wherever impermeable nodes are desired. As a consequence, at the impermeable walls, two nodes exist at the same spatial location. These two nodes are connected to elements on the opposite sides of the wall, essentially breaking the connection between two adjacent elements. The net result is an impermeable wall simulated as a 2D plane within the 3D domain. These simulations assume that the funnel walls are fully impermeable. This may not be a realistic assumption for very long-term simulations, especially for slurry walls.

GROWFLOW

GROWFLOW is an innovative permeable barrier simulation program being developed by Applied Research Associates, Inc. (Everhart, 1996) for the U.S. Air Force. The program is based on the Lagrangian smooth particle hydrodynamics (SPH) concepts traditionally used in the astrophysical simulations. SPH is a continuum dynamics solution methodology in which all hydrodynamic and history information is carried on particles. In that sense, GROWFLOW is similar to the particle-tracking codes commonly used to display the flow paths calculated by the numerical models. The particles in GROWFLOW are Lagrangian interpolation points that interact through the use of a smoothing kernel. The kernel defines a region of influence for each particle and permits approximations to spatial derivatives to be obtained without a mesh. The spatial derivatives are obtained from each particle using an explicit time-integration method.

GROWFLOW is a fully 3D, saturated-unsaturated code that can handle complex geometry. The model domain and the permeable barrier are simulated using exterior and interior flow control panels that contain and direct flow. No model grid is required. Instead, the initial particle locations serve as the integration points for spatial derivatives. The flow control panels form an impermeable boundary that restricts flow across the external model boundaries or across the internal panels that represent funnel walls. The external boundaries are simulated by assigning constant head or constant velocity source models. These source models are panels that control flow into the model domain. The flow out of the model domain is provided by a volume for the fluid to flow into; that is, the model domain is increased.

GROWFLOW input consists of the model domain parameters, the material properties, the elevation head direction, the panel locations, the saturation vs. head relationship, time-step information, saturation vs. conductivity relationship, initial locations of all particles in the system, and particle volume. In addition, information is also needed for the smoothing length (region of influence) for the particles. The output includes a listing of the input parameters, particle locations, and heads at specified time intervals. The output can be plotted to show heads as contour maps and particle movement as pathlines.

GROWFLOW is a highly innovative, flexible, and versatile code for simulation and optimization of permeable barrier systems. However, the code is still under development and several issues need to be addressed. Most importantly, the code needs to be validated against the existing analytical or numerical codes and against field data to verify its numerical accuracy. There appears to be no clear method for simulating internal sources or sinks such as wells and rivers. At many sites, these features may form a significant part of the hydrologic budgets. In addition, there appears to be no provision to check mass or volume balance in the simulations.

Funnel-and-Gate Design Model (FGDM)

FGDM is a multicomponent, steady-state, analytical program for funnel-and-gate design and cost-optimization. It was developed by Applied Research Associates (Hatfield, 1996) for the U.S. Air Force. Program input includes the initial concentrations and first-order reaction rates and the required water quality standards. These are used to determine the required residence times for water in the permeable cell. The critical residence times are used by the program along with input-plume-to-gate-width ratios to develop several funnel-and-gate designs. Finally, the cost minimization model is used to find the minimum cost design scenario based on the input unit costs for funnel walls, gate walls, reactive media, and land. The Lagrangian cost minimization is based on a modified Newton-Raphson algorithm for solution of nonlinear equations. Because the accuracy of cost minimization is based partly on the initial estimates for the minimum cost design, it is important to have a preliminary estimate of the low-cost configuration. Additional input parameters include the funnel width, hydraulic gradient, aquifer thickness, $K_{aquifer}$, gate porosity, ratio of aquifer to K_{cell}, and depth of system walls. The funnel width, the total width of funnel walls and the gate, is estimated in advance assuming a capture efficiency of 80%. For example, for a plume width of 80 ft, a funnel width of 100 ft is suggested. This assumption may need to be validated by further modeling or field studies. FGDM is a useful tool for a quick evaluation of several design scenarios in a simple setting. However, it cannot be used for complex settings such as heterogeneous media, or for evaluating the flow paths through the permeable cell.

FLONET

FLONET (Guiguer et al., 1992) is a 2D, steady-state flow model distributed by Waterloo Hydrogeologic, Inc. The program calculates potentials, streamlines, and velocities and can be used to generate flownets (maps showing flowlines and hydraulic heads) for heterogeneous, anisotropic aquifers. The funnel walls and the gate can be specified by assigning lower K to elements representing these features. The program was used by Starr and Cherry (1994) to evaluate several design scenarios for funnel-and-gate systems.

PREVIOUS MODELING STUDIES FOR PERMEABLE BARRIER APPLICATIONS

A review of the information available from prevailing sites showed that MODFLOW (McDonald and Harbaugh, 1988) in conjunction with particle tracking with codes such as MODPATH (Pollock, 1989), is the code most commonly used to simulate the permeable barriers technology. Other programs such as FLONET (Guiguer et al., 1992), FRAC3DVS (Therrien and Sudicky, 1995), FLOWPATH (Waterloo Hydrogeologic, Inc., 1996), and RWLK3D (Naymik and Gantos, 1995) also have been used at some sites. Two new codes, GROWFLOW (Everhart, 1996) and FGDM (Funnel and Gate Design Model) (Hatfield, 1996) have been developed recently for the U.S. Air Force to simulate and optimize the funnel-and-gate systems. However, these new codes have so far not been applied at any sites. The sites that used MODFLOW include the Sunnyvale, California site, Moffett Federal Airfield, California (PRC, 1996 and Battelle, 1996a), the Sommersworth Sanitary Landfill, New Hampshire, an industrial facility in Kansas, and GE Appliances, Wisconsin. FLOWPATH has been used to evaluate the design at Belfast, Northern Ireland, Fairchild Air Force Base, Washington, and the DOE Kansas City, Kansas, site. The names of simulation codes used at other sites were not readily available. The most comprehensive modeling evaluations of the permeable barrier technology are those by Starr and Cherry (1994), and Schikaze (1996). These papers evaluate the effects of various parameters on the design and performance of hypothetical funnel-and-gate configurations, although some of the conclusions are applicable to continuous reactive barriers as well.

Starr and Cherry (1994) used a two-dimensional (2-D), plan-view, steady-state flow simulation program, FLONET (Guiguer et al., 1992) to illustrate the effects of funnel-and-gate geometry (design) and reactive cell hydraulic conductivity (K_{cell}) on the size and shape of capture zone, the discharge groundwater flow volume through the gate, and the residence time in the reactive cell. Only the configurations with barriers that penetrate the entire aquifer thickness and extend into the underlying confining layer were simulated. The hanging wall systems were not simulated because they can best be described by three-dimensional (3-D) simulations. The simulated system had properties similar to those of the surficial aquifer at Canadian Forces Base Borden, Ontario, Canada. The simulated aquifer is isotropic, with homogeneous aquifer hydraulic conductivity ($K_{aquifer}$) of 28.3 feet/day and hydraulic gradient of 0.005. The funnel walls were assumed to be l-m- (3.28-feet-) thick slurry walls with K equal to 0.0028 feet/day. The K of the reactive cell was 283 feet/day, the maximum laboratory-measured value for 100 percent iron, in the base case. It should be noted that in several other modeling studies for permeable cell installations, K_{cell} values of 142 feet/day have been used for 100 percent iron. The range of values for K_{cell} indicates differences in the source of granular iron, as well as variability of the K measurement itself. A porosity of 0.33 was used for all materials. The following conclusions were made by these researchers based on the simulation of several scenarios.

- For systems with funnel walls at 180 degrees (straight funnel), the discharge through the gate and the hydraulic capture zone width increase as the funnel width increases. However, the increase in discharge is not directly proportional to funnel width. In fact, the relative discharge through the gate decreases dramatically as the funnel width increases. Relative discharge refers to the ratio of discharge through the gate to the discharge through the area in the absence of the funnel-and-gate system.

- For a constant funnel width, the absolute and relative discharge through the gate (and the capture zone width) increase with an increase in gate width. Therefore, it is desirable to have a gate as wide as practical.

- For a given funnel-and-gate design, the discharge through the gate increases with increase in K_{cell} relative to the $K_{aquifer}$. However, there is relatively little increase in discharge when the K_{cell} is more than 10 times higher than the $K_{aquifer}$. This implies that while a reactive cell conductivity higher than the $K_{aquifer}$ is desirable, K_{cell} does not have to be much higher than $K_{aquifer}$. This is a useful result, because the large grain sizes required for very high-K_{cell} values would result in a low total surface area for reactions and lower residence times.

- For all orientations to the regional flow gradient, the maximum absolute discharge occurs at apex angles (the angles between the two funnel walls) of 180 degrees (straight barrier). However, for apex angles between 127 and 233 degrees there is little effect on discharge. Outside this range, the discharge drops rapidly. This implies that there is no significant advantage of a slightly angled funnel-and-gate system over a straight barrier and vice versa. Sharper funnel angles may, however, reduce discharge.

- For all apex angles, the maximum discharge occurs when the funnel is perpendicular to the regional flow gradient.

- The groundwater flow models can be used effectively to design the funnel-and-gate systems at sites with special design requirements due to complex flow fields, seasonal fluctuations, or access restrictions. These may include systems with angled funnels, multiple gates, asymmetrical funnels, or U-shaped funnel-and-gates.

- A balance between maximizing the capture zone of the gate and maximizing the residence times of contaminated water in the gate should be achieved. In general, the discharge and residence times are inversely proportional. The residence time can generally be increased without affecting the capture zone by increasing the width of the gate.

Schikaze (1996) used FRAC3DVS code to examine 3-D groundwater flow in the vicinity of a partially penetrating (hanging wall) funnel-and-gate system for 16 different combinations of parameters. All simulations were for steady-state, fully saturated groundwater flow. The 16 simulations consisted of variations in four dimensionless parameters: the ratio of K_{cell} to $K_{aquifer}$; the ratio of width of a single funnel wall to the depth of the funnel-and-gate; the ratio of total funnel wall width to the gate width; and the hydraulic gradient. The following conclusions were drawn from these simulations:

- Absolute discharge through the gate increases as the hydraulic gradient increases. However, there is almost no effect of hydraulic gradient on the relative discharge or on the size of the relative capture zone (hydraulic capture zone width ÷ total width of funnel-and-gate).

- For higher values of K_{cell} versus $K_{aquifer}$, there is an increase in absolute and relative discharge through the gate as well as in the relative size of the capture zone. Thus, a higher K_{cell} tends to draw more flow towards the gate.

- Higher values for the ratio of width of the single funnel wall (one wing) to the depth of the funnel-and-gate system result in lower absolute and relative discharge, and in smaller capture zones. This is due to the fact that in cases of wide but shallow funnel walls, there is an increase in the flow component that is diverted under the barrier rather than through the gate.

- Higher values for the ratio of total funnel wall width to the width of the gate result in higher absolute discharge but lower relative discharge and smaller hydraulic capture zones. This implies that, for wider funnel walls, the increase in the discharge through the gate is not proportional to the increase in the funnel wall area.

APPENDIX B-2
ILLUSTRATION OF THE HYDROLOGIC MODELING APPROACH FOR PERMEABLE BARRIER APPLICATION

The following methodology serves as an illustration of the permeable barrier design modeling approach for homogeneous and heterogeneous aquifers. Modeling may be used to design the location, configuration, and dimensions of the permeable barrier, as well as to develop a performance monitoring plan.

Homogeneous Aquifers

MODFLOW can be used to develop a steady-state numerical approximation of the groundwater flow field and to calculate flow budgets through the gate. Particle tracking techniques under advective flow conditions only can be used to delineate capture zones and travel times in the vicinity of the funnel and gate. RWLK3D (Prickett et al., 1981) or any similar particle tracking code could be used to simulate particle pathways. The model simulations can be performed to aid in both the design phase and the evaluation phase of permeable barrier systems for the containment and remediation of contaminated groundwater. These simulations can build upon previous modeling efforts conducted by Starr and Cherry (1994). Specific objectives can include determining how changes in gate conductivity over time affected capture zone width, retention times for groundwater moving through the gate, and flow volumes through the gate.

The model domain and grid size are typically determined based on the site-specific conditions. The primary criteria are that the domain should be large enough so that the boundary conditions do not affect flow in the vicinity of the permeable barrier. Further, the model cell size in the vicinity of the permeable barrier should be small enough to provide sufficient resolution for retention time calculations. The funnel-and-gate configuration modeled in this illustration is a pilot barrier at a U.S. Navy base in California (see Figure B-1). The funnel consists of two 20-foot lengths of sheet piling oriented perpendicular to flow on either side of a 10-foot by 10-foot reactive cell representing the gate. The reactive cell is bounded on its sides by 10-foot lengths of sheet piling. The gate itself consists of 2 feet of 3/4-inch pea gravel located on both the upgradient and downgradient ends of the reactive cell, which has a 6-foot flowthrough thickness.

For this model of a funnel-and-gate system, the domain consisted of a single layer that is 500 feet long and 300 feet wide. The grid has 98 rows and 106 columns resulting in a total of 10,388 nodes. Grid nodes are 10 feet by 10 feet at their maximum (in the general domain area) and 0.5 foot by 0.5 foot in the region of the gate itself. Specified head nodes were set along the first and last rows of the model to establish a gradient of 0.006. No flow conditions were set along the first and last columns of the model.

The funnel (sheet piling) was simulated as a horizontal flow barrier having a K of 2.0 x 10^{-6} feet/day. For the continuous reactive barrier configuration, the funnel may be excluded from the model. The pea gravel was assigned a K of 2,830 ft/d. The reactive cell consisting of granular iron was assigned a K of 283 ft/d, the maximum laboratory-measured value for 100% iron. It should be noted that in some modeling studies (e.g., Thomas et al., 1995), a reactive cell with K of 142 ft/d has been used for 100% iron. In general, the K value for the reactive medium should be determined from laboratory permeability testing. Porosity was held constant at 0.30 for all materials in each of the simulations.

For this illustration, simulated $K_{aquifer}$ was varied among 0.5, 1, 2, 5, 10, 20, 50, and 100 ft/d to represent low- and high-permeability aquifers. Once this base scenario was established, simulations were conducted to evaluate reductions in K_{cell} over time that could potentially be caused by buildup of precipitates. To determine the effects of decreased permeability of the gate over a period of operation,

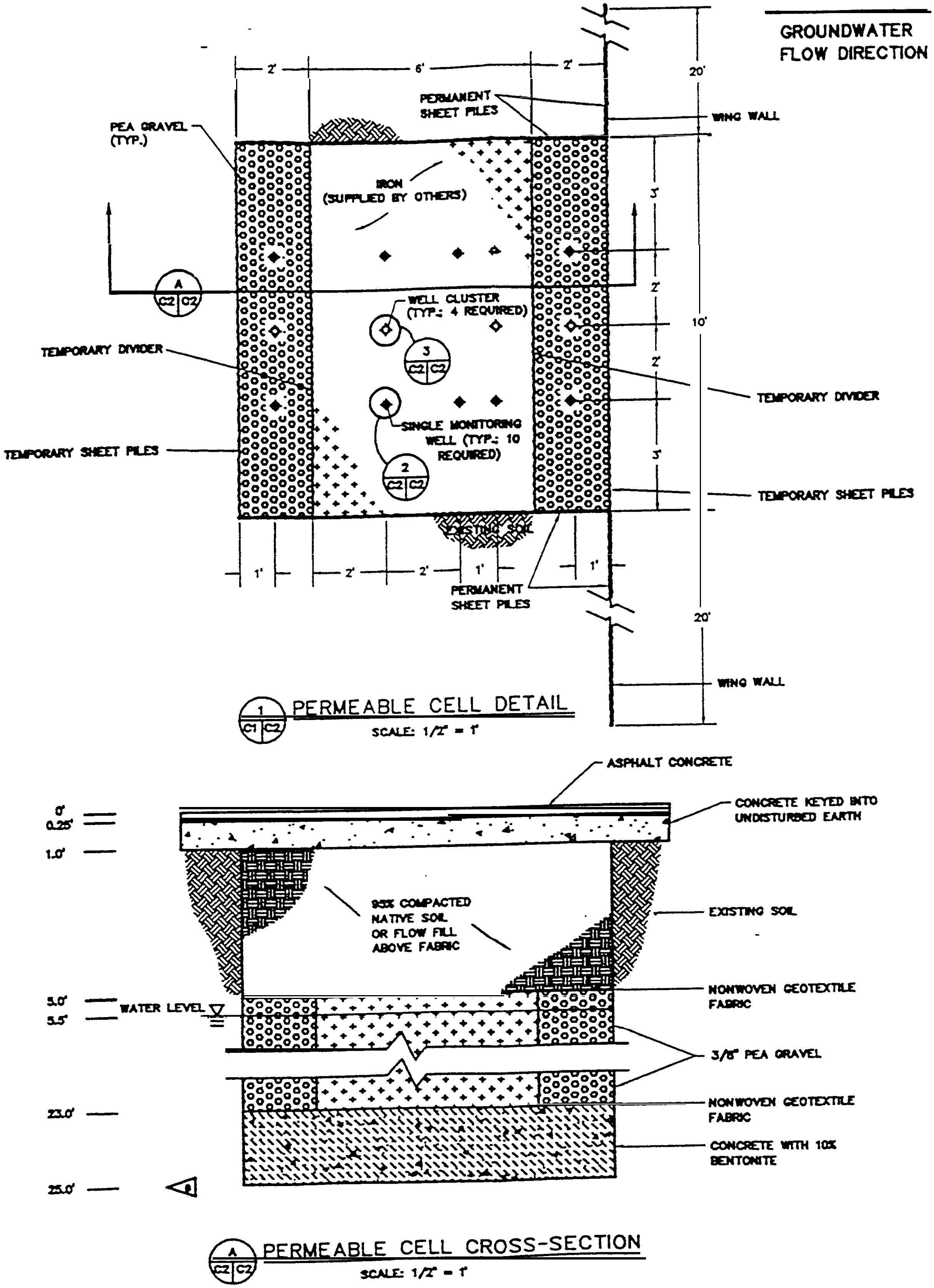


Figure B-l. Pilot-Scale Funnel-and-Gate System Installed at Moffett Federal Airfield, CA (Courtesy of Naval Facilities Engineering Service Center [NFESC] and PRC, Inc., 1996)

K_{cell} was reduced in 10 percent increments from the initial 283 ft/d to 28.3 ft/d for each value of $K_{aquifer}$. An additional set of simulations were performed with K_{cell} reduced by 95% to 14.15 ft/d, resulting in a total of 11 simulations for each value of $K_{aquifer}$. For each individual simulation, a single value for $K_{aquifer}$ was used. The effects of geologic heterogeneities were not considered in these simulations. The results from the 88 simulations were used to evaluate the impact of variations in K_{cell} and $K_{aquifer}$ on capture zone width, flow volumes, and travel times (retention time) through the gate.

Table B-1 lists the model run number, gate conductivity, aquifer conductivity, ratio of reactive cell to aquifer conductivity, capture zone width, residence time within the reactive cell, and groundwater discharge through the gate. Capture zone width in each of the simulations was determined by tracking particles forward through the gate. Two hundred particles (1 particle every 0.5 feet) were initiated along a 100-foot-long line source upgradient from the barrier. The locations of the flow divides between particles passing through the gate and those passing around the ends of the funnel were used to determine capture zone width. Residence time within the gate for each simulation was determined from the length of time required for the particles to pass through the reactive cell. Figure B-2 illustrates the determination of flow divides and travel times for simulation number 57, which had an aquifer conductivity of 20 ft/d and a reactive cell conductivity of 283 ft/d. Particle pathlines have been overlain upon the calculated water-table surface. Particle pathlines and intermediate time steps within the reactive cell are also shown. In some cases, there may be significant variation in residence times at the edges of the reactive cell and at its center. For example, Vogan et al. (1994) showed that simulated residence times in a funnel-and-gate system (with caisson gates) varied from 29 hours at the edges to 82 hours in the center of the reactive cell.

Discharge through the gate was determined from the MODFLOW-calculated, cell-by-cell flow file using the MODUTILITY code zone budget (Harbaugh, 1990). Correlations between $K_{aquifer}$ and K_{cell}, retention time, discharge, and capture zone width can be determined by plotting the results of the 88 simulations against one another. Some basic relationships are readily apparent.

Figure B-3 illustrates the correlation between $K_{aquifer}$, retention time, and discharge through the gate. There is an inverse relationship between $K_{aquifer}$ and retention time. As aquifer conductivity increases, the retention time within the gate decreases. As aquifer conductivity increases, the total discharge through the gate increases. Finally, Figure B-3 shows a very strong inverse correlation between the total discharge through the gate and the retention time within the gate. Therefore, aquifers having high hydraulic conductivities may require greater flow through thickness of gate to meet residence time requirements so that contaminant levels can be reduced to regulatory limits.

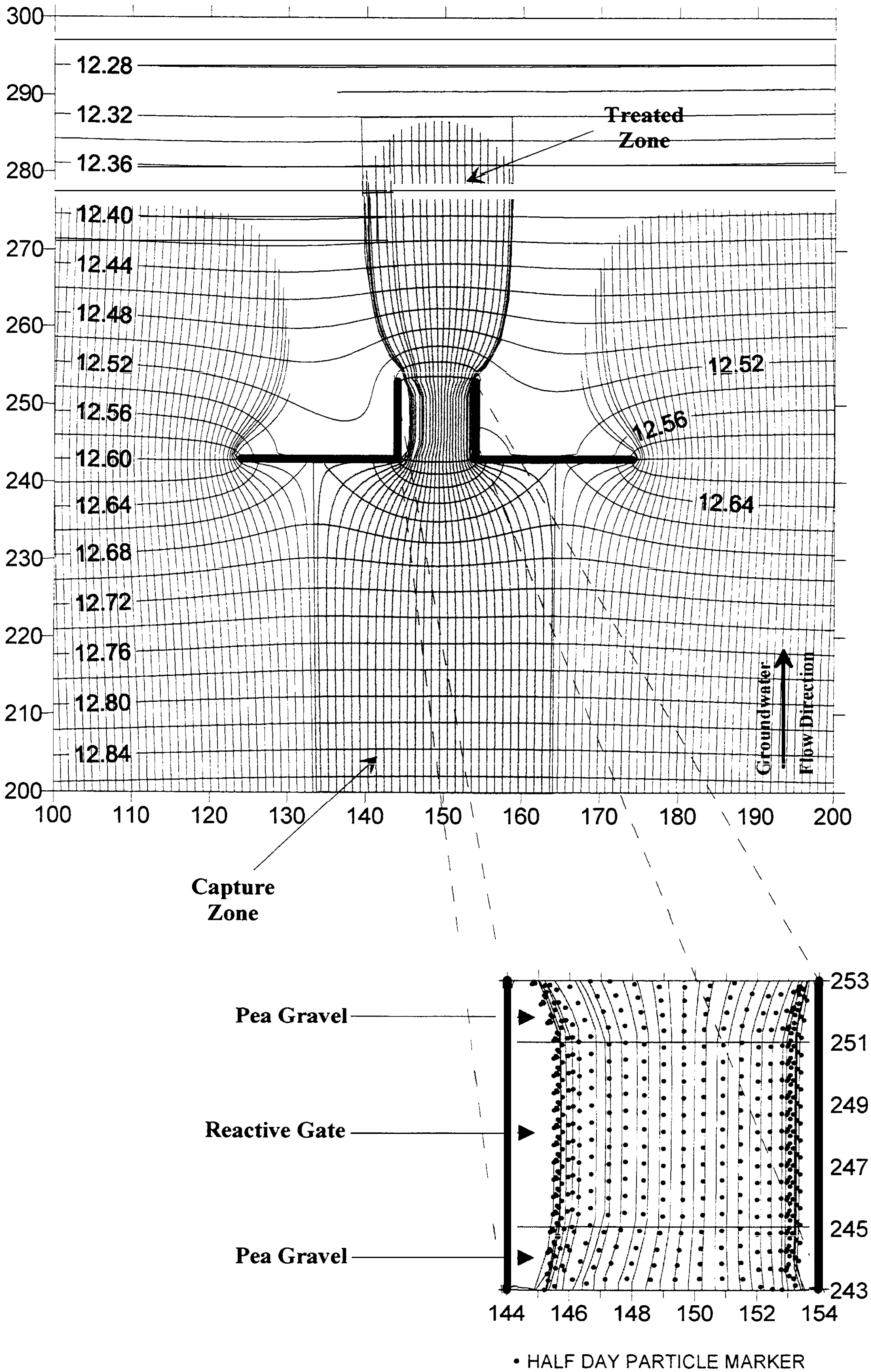
The conductivities of both the aquifer and the reactive cell were plotted against capture zone width. A general correlation exists between an increase in K (and discharge through the gate) and capture zone width. As K increased, the capture zone width generally increased. However, the capture zone width appears to be more sensitive to the length of the funnel walls and was generally observed to occur at just over half of the funnel wall length on either side of the gate. Capture zone widths ranged from roughly 0.2 to 2 feet beyond the midpoint of the funnel wall. Figure B-4 is a plot showing the reduction in discharge (due to potential buildup of precipitate) through the gate that results from decreasing K_{cell} at aquifer conductivities of 0.5, 10, and 100 ft/d. In each of the plots shown in Figure B-4, K_{cell} decreases from 283 ft/d to 14.15 ft/d. Reductions in K_{cell} were simulated to represent the potential clogging of the reactive cell by precipitation. The percent decline in discharge through the gate was determined for each decline in K_{cell}. When aquifer conductivity is 0.5 ft/d, the reactive cell conductivity is much greater than the aquifer conductivity for each of the 11 simulations performed, and the percent decline in discharge

Table B-1. Summary of Funnel-and-Gate Model Runs

Run #	K_{gate} (ft/day)	$K_{aquifer}$ (ft/day)	Kg:Kaq	Capture Width (ft)	Discharge Cu ft/day	Residence Time (days)	Relative Discharge
1	283	0.1	2830.00	NA	NA	NA	NA
2	283	0.5	566.00	34	2.356	219.0	1.000
3	255	0.5	509.40	NA	2.356	220.0	1.000
4	226	0.5	452.80	NA	2.355	218.0	1.000
5	198	0.5	396.20	NA	2.355	219.0	1.000
6	170	0.5	339.60	NA	2.354	220.0	0.999
7	142	0.5	283.00	NA	2.354	219.0	0.999
8	113	0.5	226.40	NA	2.353	218.0	0.999
9	85	0.5	169.80	NA	2.352	220.0	0.998
10	57	0.5	113.20	NA	2.350	220.0	0.998
11	28	0.5	56.60	NA	2.344	220.0	0.995
12	14	0.5	28.30	NA	2.334	NA	0.991
13	283	1	283.00	32.75	4.732	107.0	1.000
14	255	1	254.70	NA	4.732	107.5	1.000
15	226	1	226.40	NA	4.730	107.5	1.000
16	198	1	198.10	NA	4.729	107.5	0.999
17	170	1	169.80	NA	4.727	107.5	0.999
18	142	1	141.50	NA	4.725	107.5	0.998
19	113	1	113.20	NA	4.721	107.5	0.998
20	85	1	84.90	NA	4.716	107.5	0.997
21	57	1	56.60	NA	4.705	108.0	0.994
22	28	1	28.30	NA	4.672	108.5	0.987
23	14	1	14.15	NA	4.603	110.0	0.973
24	283	2	141.50	NA	9.475	52.5	1.000
25	255	2	127.35	NA	9.472	52.5	1.000
26	226	2	113.20	NA	9.468	52.5	0.999
27	198	2	99.05	NA	9.462	52.5	0.999
28	170	2	84.90	NA	9.455	52.5	0.998
29	142	2	70.75	NA	9.446	52.5	0.997
30	113	2	56.60	NA	9.432	53.0	0.995
31	85	2	42.45	NA	9.408	53.0	0.993
32	57	2	28.30	NA	9.362	53.5	0.988
33	28	2	14.15	NA	9.223	54.5	0.973
34	14	2	7.08	NA	8.954	56.0	0.945
35	283	5	56.60	32.17	23.613	21.0	1.000
36	255	5	50.94	NA	23.593	20.9	0.999
37	226	5	45.28	NA	23.568	21.0	0.998
38	198	5	39.62	NA	23.535	21.1	0.997
39	170	5	33.96	NA	23.493	21.1	0.995
40	142	5	28.30	NA	23.432	21.1	0.992
41	113	5	22.64	NA	23.344	21.3	0.989
42	85	5	16.98	NA	23.197	21.4	0.982
43	57	5	11.32	NA	22.909	21.6	0.970
44	28	5	5.66	NA	22.082	22.6	0.935
45	14	5	2.83	NA	20.597	24.0	0.872
46	283	10	28.30	32.17	46.407	10.6	1.000
47	255	10	25.47	32.17	46.328	10.6	0.998

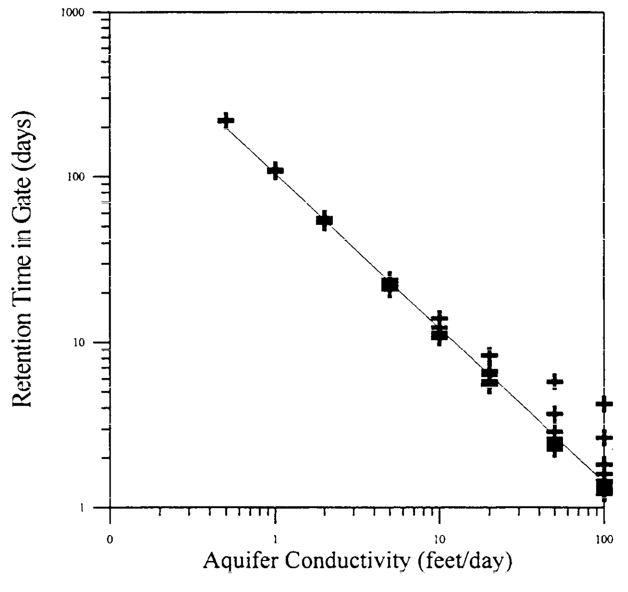
Table B-1. Summary of Funnel-and-Gate Model Runs (Continued)

Run #	K_{gate} (ft/day)	$K_{aquifer}$ (ft/day)	Kg:Kaq	Capture Width (ft)	Discharge Cu ft/day	Residence Time (days)	Relative Discharge
48	226	10	22.64	32.17	46.169	10.8	0.995
49	198	10	19.81	32.33	46.040	10.7	0.992
50	170	10	16.98	32.33	45.870	10.9	0.988
51	142	10	14.15	32.5	45.628	10.9	0.983
52	113	10	11.32	31.5	45.274	11.0	0.976
53	85	10	8.49	31.67	44.763	11.0	0.965
54	57	10	5.66	31.83	43.566	11.4	0.939
55	28	10	2.83	32.17	40.562	12.3	0.874
56	14	10	1.42	NA	35.630	13.9	0.768
57	283	20	14.15	31.81	91.493	5.4	1.000
58	255	20	12.74	NA	91.239	5.4	0.997
59	226	20	11.32	NA	91.331	5.5	0.998
60	198	20	9.91	NA	89.890	5.6	0.982
61	170	20	8.49	NA	89.262	5.6	0.976
62	142	20	7.08	NA	88.379	5.6	0.966
63	113	20	5.66	NA	86.708	5.7	0.948
64	85	20	4.25	NA	84.126	5.8	0.919
65	57	20	2.83	NA	78.681	6.3	0.860
66	28	20	1.42	NA	73.403	6.7	0.802
67	14	20	0.71	NA	59.502	8.3	0.650
68	283	50	5.66	31.5	221.445	2.3	1.000
69	255	50	5.09	NA	219.770	2.3	0.992
70	226	50	4.53	NA	217.730	2.3	0.983
71	198	50	3.96	NA	215.185	2.4	0.972
72	170	50	3.40	NA	211.925	2.4	0.957
73	142	50	2.83	NA	207.005	2.4	0.935
74	113	50	2.26	NA	200.755	2.5	0.907
75	85	50	1.70	NA	190.560	2.6	0.861
76	57	50	1.13	NA	173.695	2.9	0.784
77	28	50	0.57	NA	136.155	3.7	0.615
78	14	50	0.28	NA	94.409	5.8	0.426
79	283	100	2.83	30.38	410.105	1.3	1.000
80	255	100	2.55	NA	404.240	1.2	0.986
81	226	100	2.26	NA	397.135	1.2	0.968
82	198	100	1.98	NA	388.355	1.3	0.947
83	170	100	1.70	NA	377.240	1.3	0.920
84	142	100	1.42	NA	362.735	1.4	0.884
85	113	100	1.13	NA	343.060	1.5	0.837
86	85	100	0.85	NA	314.455	1.6	0.767
87	57	100	0.57	NA	268.935	1.8	0.656
88	28	100	0.28	NA	188.075	2.7	0.459
89	14	100	0.14	NA	116.935	4.2	0.285
90	283	200	1.42	NA	NA	NA	NA

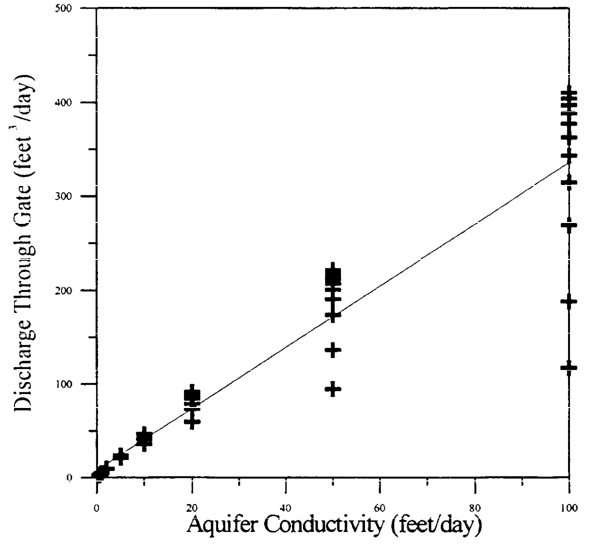


ure B-2. Simulated Particle Pathlines Overlain upon Water Table Including Zoomed in View of Gate Area

A) K $_{aquifer}$ versus Retention Time



B) K $_{aquifer}$ versus Discharge



C) Retention Time versus Discharge

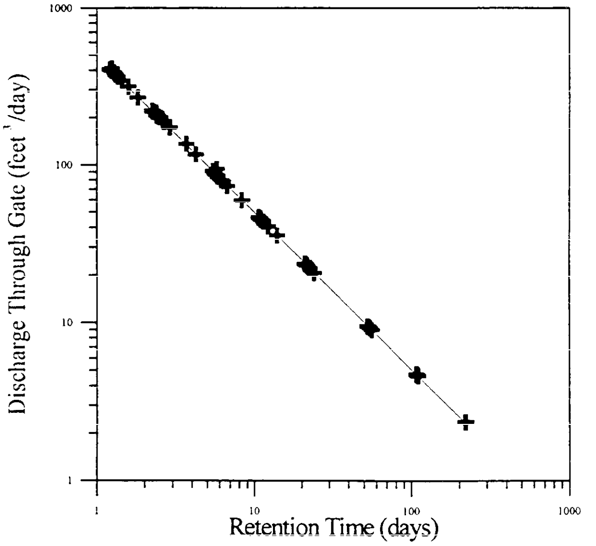


Figure B-3. Correlation Between K$_{aquifer}$, Discharge, and Travel Time Through the Gate for a Homogeneous, One-Layer Scenario

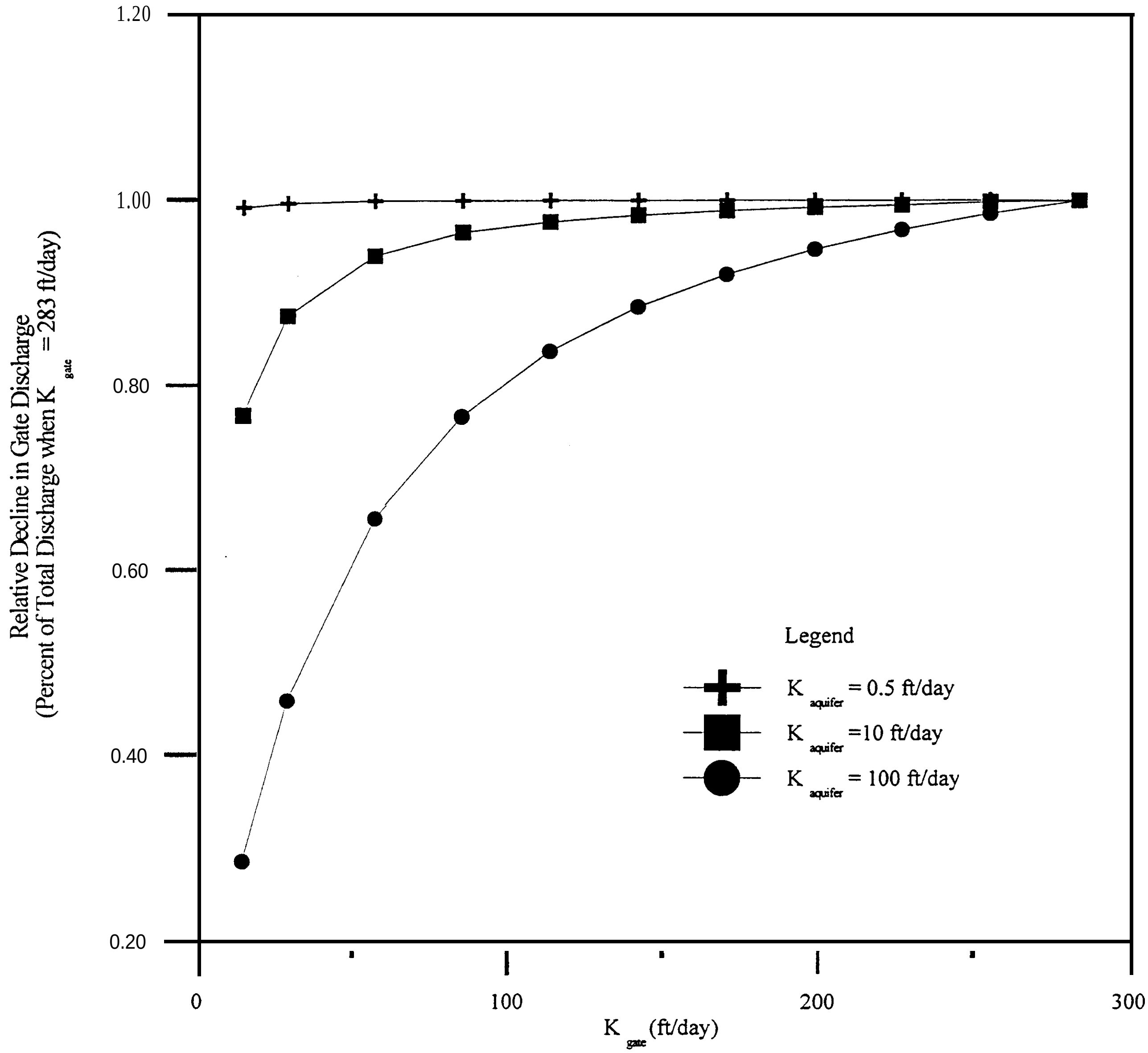


Figure B-4. Correlation Between K_{cell} and Discharge at $K_{aquifer}$ of 0.5, 10, and 100 feet per day K_{cell} Varied Between 283 and 14.15 feet per day

in only a 1 percent decline in the discharge through the gate. As aquifer conductivity was increased, a larger reduction in discharge through the gate occurred as the reactive cell conductivity decreased. For aquifer conductivities of 10 and 100 ft/d, discharge through the gate decreased by roughly 27 and 71 percent, respectively, over the same decline in gate conductivity. In both cases, the ratio of K_{cell} to $K_{aquifer}$ approaches or becomes less than 1 as K_{cell} decreases. Therefore, the effects of precipitate buildup in the reactive cell are likely to be felt earlier in high-permeability aquifers. However, as discussed below, there is considerable leeway before such effects are noticed.

Figure B-5 is a plot of the ratio of K_{cell} to $K_{aquifer}$ versus discharge through the gate for the 88 simulations. The plot indicates that declines in reactive cell conductivity due to clogging have very little influence on the volume of groundwater passing through the gate as long as the reactive cell conductivity is roughly 5 times the conductivity of the aquifer. In these instances, discharge through the gate remained at roughly 95 percent of the simulated discharge when the gate conductivity was 283 ft/d. Because discharge is relatively unaffected, residence times and capture zone width will remain relatively unchanged for a given aquifer conductivity. As the ratio between K_{cell} and $K_{aquifer}$ declines below 5, the relative decrease in discharge becomes greater and results in decreased capture zone widths and increased retention times. Thus, as long as the hydraulic conductivity of a freshly installed reactive cell is designed to be one or two orders of magnitude greater than the hydraulic conductivity of the aquifer, there is considerable flexibility for precipitates to build up without significantly affecting the hydraulic capture zone.

Heterogeneous Aquifers

Most modeling studies at previous permeable barrier sites were based on the assumption that the aquifer sediments in the vicinity of the permeable barrier are homogeneous. However, at many sites, there may be strong heterogeneity in the sediments. This heterogeneity develops mainly due to the variations in depositional environments of the sediments. The general implications of heterogeneity are that more detailed site characterization is required and the models are more complex. The symmetrical capture zones seen in cases of homogeneous sediments become asymmetrical and difficult to predict without detailed characterization and modeling.

Examples of the effect of heterogeneity on the flow paths and capture zones can be seen from the modeling work conducted in support of the design and performance monitoring for the Moffett Federal Airfield (MFA) Site (Battelle, 1996b and PRC, 1996) and the Elizabeth City, NC site (Puls et al., 1995). Groundwater flow modeling for the MFA pilot barrier showed that the presence of heterogeneities due to multiple subsurface channels (strata) causes the capture zones to be substantially asymmetrical. Figure B-6 is a simulated flow path diagram showing the result of backward particle tracking for 25 days with particles starting from the funnel area in model layers 1 through 4 at the funnel location. The reactive cell is present in layers 2, 3, and 4 of the model.

The most striking observation from this figure is that the capture zone for a permeable barriers at a heterogeneous site is highly asymmetrical and there is a significant difference in the residence time at different depth levels. For example, there is almost no movement of particles in 25 days in layers 1 and 2. In layer 3, the particle movement is very fast directly upgradient of the gate but very slow upgradient of the funnel walls. In layer 4, the particle movement is very fast upgradient of the gate in the west funnel wall but still very slow upgradient of the east funnel. These differences in particle velocities and resulting irregularities in the capture zones are because the lower part of the reactive cell is located in a high-permeability sand channel, whereas the funnel walls and the upper portion of the reactive cell are located in the lower conductivity interchannel deposits. The location of sand channels at the site

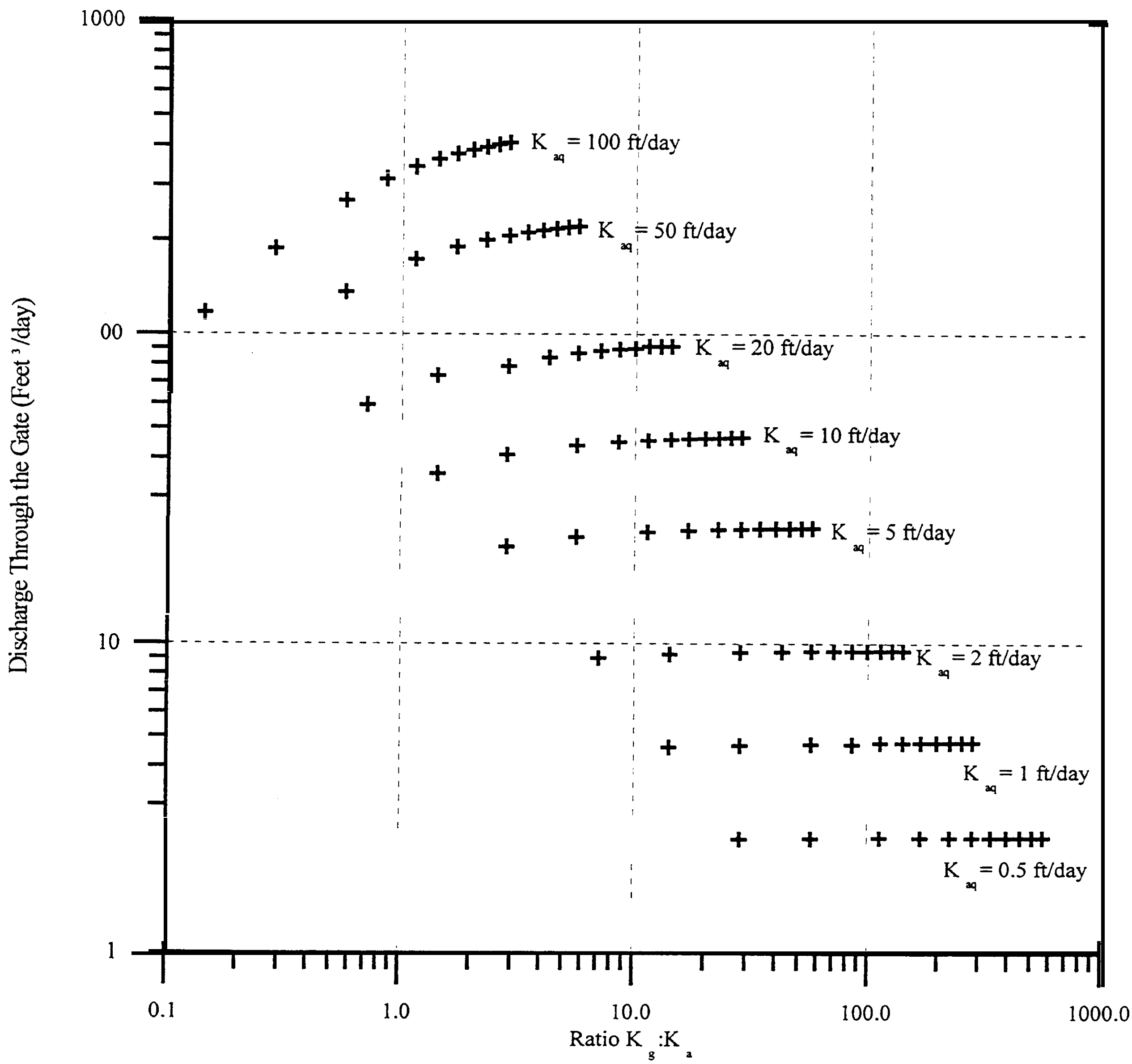


Figure B-5. Correlation Between Ratio of K_{cell} to $K_{aquifer}$ Versus Discharge Through the Gate for a Homogeneous, One-Layer Scenario

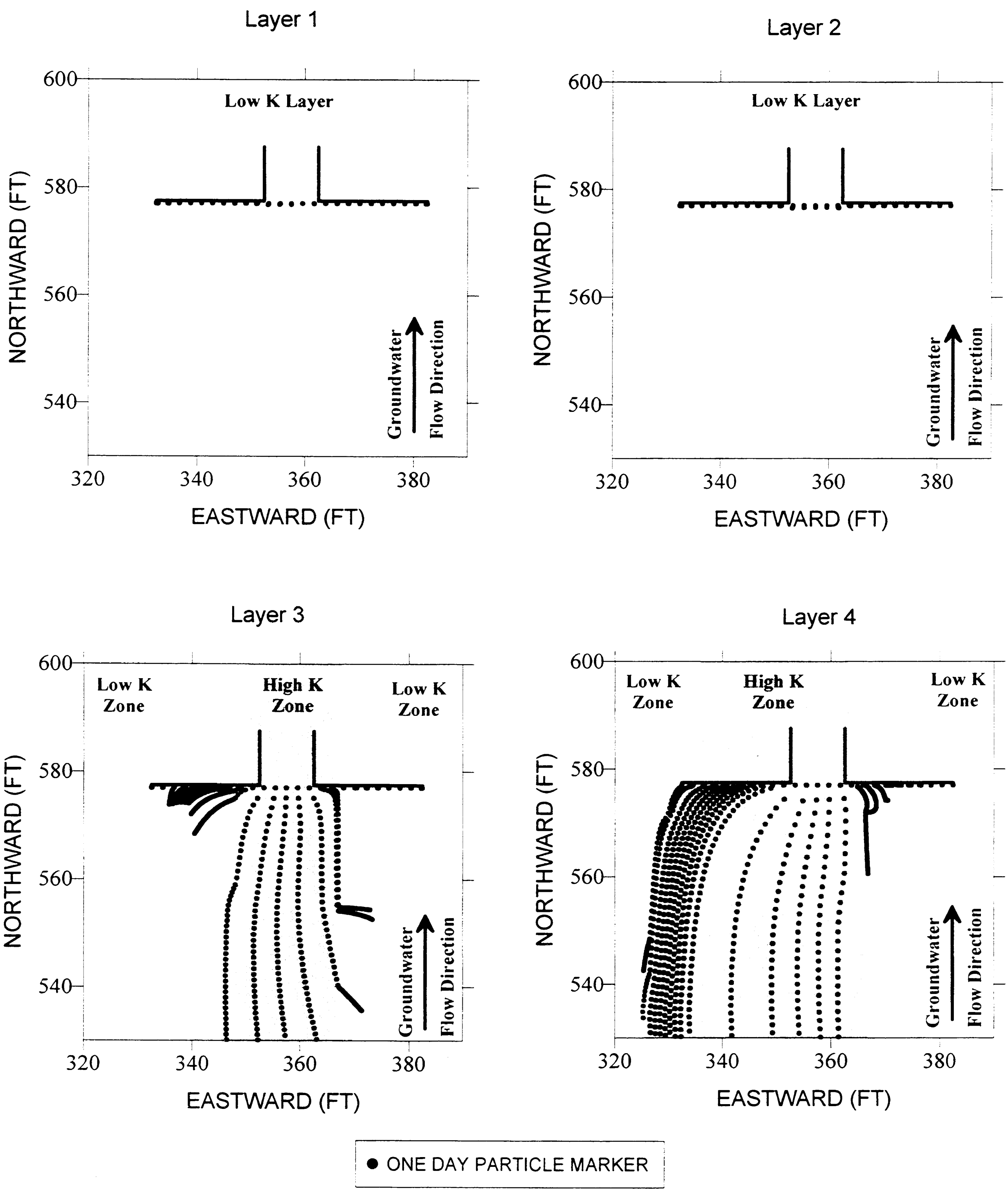


Figure B-6. MFA Funnel-and-Gate Backward Particle Tracking Showing the Effect of Heterogeneity on Capture Zones (Battelle, 1996b)

was determined based on the preexisting base-wide site characterization maps and from site-specific CPT data.

At the Elizabeth City, NC Site (Puls et al., 1995), the site geology is characterized by complex and variable sequences of surficial sands, silts, and clays. Groundwater flow velocity is extremely variable with depth, with a highly conductive layer at approximately 12 to 20 feet below ground surface. The reactive metal zone was emplaced in this sand channel (Figure B-7).

These examples illustrate the need for placing the reactive cell in a zone of high conductivity that forms a preferential pathway for most of the flow and contaminant transport through the aquifer. Additionally, the dependence of capture zones on aquifer heterogeneities illustrates the need for detailed site characterization prior to permeable barrier placement.

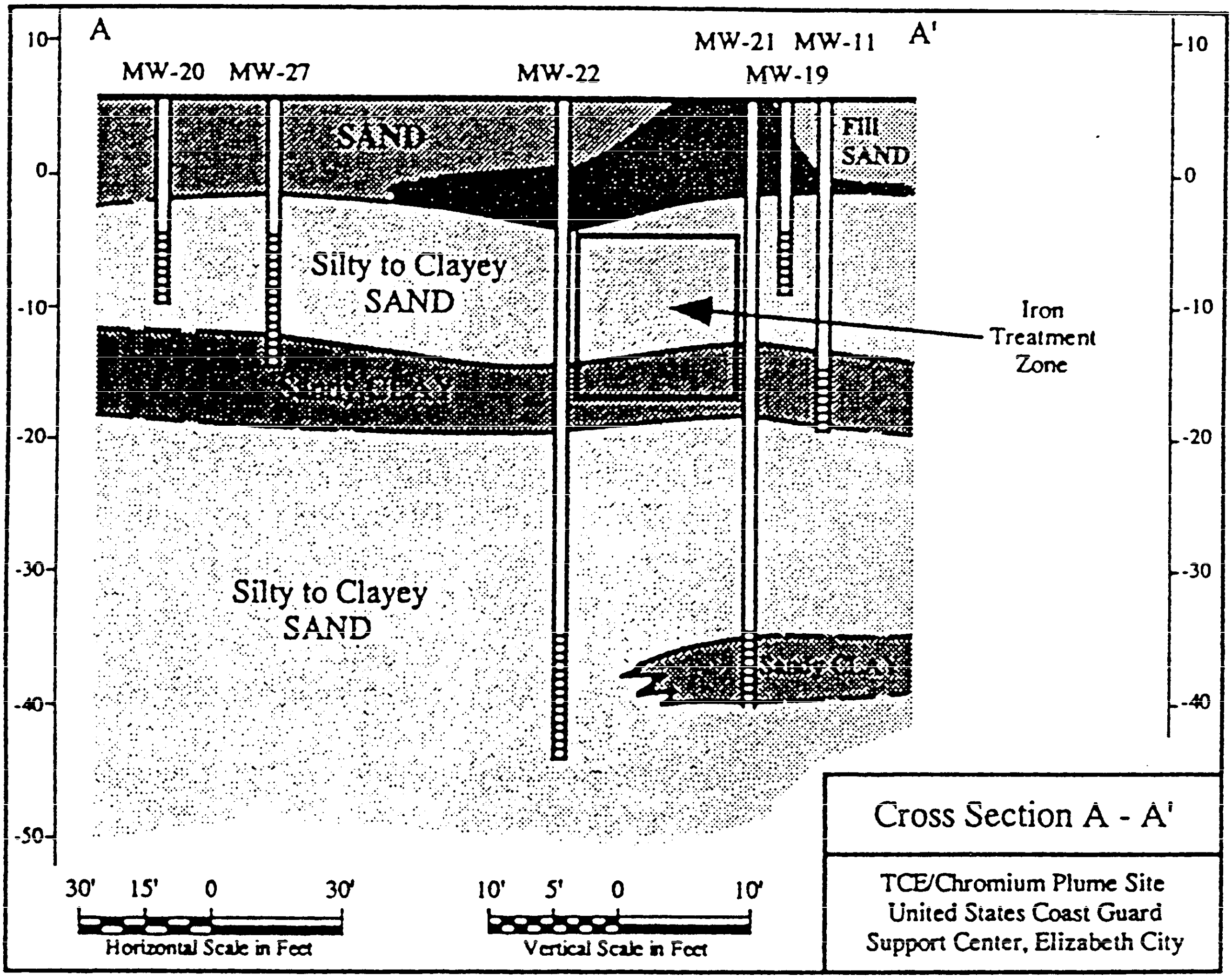


Figure B-7. Location of Reactive Cell in a Sand Channel (Source: Puls et al., 1995)